



LAWRENCE
LIVERMORE
NATIONAL
LABORATORY

Kinetic theory and Vlasov simulation of nonlinear ion acoustic waves in multi-ion species plasmas

T. D. Chapman, R. L. Berger, S. Brunner, E. A. Williams

January 2, 2013

Physical Review Letters

Disclaimer

This document was prepared as an account of work sponsored by an agency of the United States government. Neither the United States government nor Lawrence Livermore National Security, LLC, nor any of their employees makes any warranty, expressed or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States government or Lawrence Livermore National Security, LLC. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States government or Lawrence Livermore National Security, LLC, and shall not be used for advertising or product endorsement purposes.

Kinetic theory and Vlasov simulation of nonlinear ion acoustic waves in multi-ion species plasmas

T. Chapman,^{1,*} R. L. Berger,¹ S. Brunner,² and E. A. Williams¹

¹*Lawrence Livermore National Laboratory, P.O. Box 808, Livermore, CA 94551, USA*

²*Centre de Recherches en Physique des Plasmas, Association EURATOM-Confédération Suisse, Ecole Polytechnique Fédérale de Lausanne, CRPP-PPB, CH-1015 Lausanne, Switzerland*

(Dated: December 11, 2012)

The theory of damping and nonlinear frequency shifts from particles resonant with the Ion Acoustic Waves (IAWs) are presented for multi-ion species plasma and compared to driven wave Vlasov simulations. Multi-species plasmas may support multiple IAW modes, broadly classified as fast and slow by their phase velocity relative to the constituent ion thermal velocities. Which mode is the least damped, and thus more readily driven, is dependent on the ion to electron temperature ratio, T_i/T_e . At $T_i/T_e \gtrsim 0.2$, as is expected in the latter stages of current fusion-relevant long pulse experiments, the least damped mode is the slow mode. The lighter ion species of the slow mode is found to make no significant contribution to the IAW frequency shift despite typically being the dominant contributor to the Landau damping.

PACS numbers:

In long pulse laser plasma interaction experiments, inverse bremsstrahlung heating and electron transport raise electron temperatures in underdense plasma to $\gtrsim 1$ keV [1]. From the ablator of NIF ignition hohlraums, an underdense multi-ion species plasma with mm scale lengths is formed over 16–18 ns [1]. This plasma supports multiple Ion Acoustic Wave (IAW) modes associated with different oscillation phases of the constituent plasma species, many observations of which have been made experimentally [2], with damping rates sensitive to the ion to electron temperature ratio, T_i/T_e . For typical ablator materials, the electron-ion temperature equilibration rate is ~ 3 ns, giving ample time for T_i to approach T_e , in contrast to sub-nanosecond interactions which comprise the majority of Stimulated Brillouin Scattering (SBS) experiments [2].

Via SBS, IAWs may grow and scatter significant laser energy away from its desired path in ICF experiments, impeding the ablation process necessary for ignition. The question of which IAW mode is least damped thus becomes of great importance in understanding the behaviour of SBS. CH is the standard ablator for NIF ignition capsules owing to its low atomic number, high density and a host of manufacturing considerations [3]. As T_i approaches T_e , the least damped mode is the “slow mode” (defined later), with phase velocity close to the H ion thermal velocity [4]; this is true for the slow mode of CH for all physically relevant T_i/T_e , but is also applicable for C/H number fractions as low as ~ 0.01 and for the slow modes of a diverse range of plasmas (e.g., Xe-H mixtures with Xe/H number fractions greater than ~ 0.1).

This Letter provides the first examination of the complex nonlinear behaviour of multi-ion species IAWs as the wave amplitude and electron-to-ion temperature ratio are varied. Previously, we showed for a single-ion species

plasma the importance of including the kinetic contribution of the electrons and harmonic generation to describe IAWs driven to a nonlinear BGK-like equilibrium state [5]. There, we found that the ions of charge Z provided the dominant damping in the linear state and the dominant contribution to the nonlinear frequency shift in the BGK-like state if $ZT_e/T_i \lesssim 10$. Based on these results, one might expect for a CH plasma that the H ions with $Z = 1$ would provide the dominant frequency shift in the nonlinear state. However, the theory of nonlinear frequency shifts for fast and slow modes presented here and Vlasov simulations show that the H ions play almost no role in the frequency shift of the slow mode. It will also be shown by comparison of theory and Vlasov simulations that the distribution function for all species is best represented by an adiabatic one (to be specified clearly later), in contrast to non-adiabatic ion and fluid electron models used and simulations performed previously (e.g., Refs. [6, 7]). In the regime considered here, both harmonic generation and kinetic wave-particle interactions are required to achieve quantitative agreement between theoretical models of the nonlinear IAW frequency and Vlasov simulations. While we address the physically relevant case of CH, these findings are applicable to many multi-species plasmas.

We consider a neutral, fully-ionized CH plasma (50:50 mix). The ion species in multi-ion modes are typically characterized by their thermal velocities relative to the phase velocity v_ϕ of an IAW of wave number k and frequency ω , where $v_\phi = \text{Re}[\omega]/k$. An ion species of mass m_i and temperature T_i with thermal velocity $v_{th,i} = \sqrt{T_i/m_i}$ is regarded as heavy when $v_{th,i} < v_\phi$ and light when $v_{th,i} > v_\phi$. Similarly, IAW modes are loosely classified as “fast” when $v_\phi > v_{th,1,2}$ and “slow” when $v_{th,1} > v_\phi > v_{th,2}$ (in our example, species 1 is H and 2 is C). The properties of an IAW mode, including its

phase velocity and Landau damping, are dependent on the relative fractions and mass ratios of the ion species and on T_i/T_e . Across the parameter space of interest, the ion and phase velocities of the fast mode of CH are all well separated. The so-called slow mode, however, has a phase velocity that is only weakly dependent on T_i/T_e such that $v_\phi \sim v_{th,H}$, making conventional treatments of the slow mode difficult.

The multi-species, linear kinetic dispersion relation for one dimensional (1D) longitudinal plasma waves in a non-magnetized, homogeneous plasma is given by,

$$\epsilon_L(\omega, k) = 1 + \sum_{\text{species}} \chi_j = 0, \quad \chi_j = \frac{1}{(k\lambda_{D,j})^2} W\left(\frac{\omega}{kv_{th,j}}\right), \quad (1)$$

where χ_j is the species j (electron, H ion or C ion) susceptibility with density N_j , charge number \tilde{Z}_j , temperature T_j and mass m_j , for which $\lambda_{D,j}^2 = v_{th,j}^2/\omega_{p,j}^2$, $v_{th,j}^2 = T_j/m_j$, and $\omega_{p,j}^2 = N_j \tilde{Z}_j^2 e^2/m_j \epsilon_0$. e is the magnitude of the electron charge and ϵ_0 is the permittivity of free space. W is the dispersion function,

$$W(\bar{z}_j) = \frac{1}{\sqrt{2\pi}} \int d\bar{v}_j \frac{\bar{v}_j}{\bar{v}_j - \bar{z}_j} \exp(-\bar{v}_j^2/2), \quad (2)$$

where $\bar{v}_j = v/v_{th,j}$, $\bar{z}_j \equiv v_\phi/v_{th,j}$ and a Maxwellian velocity distribution for all species is assumed. The dispersion relation $\epsilon(\omega, k) = 0$ relates ω to k for any given electrostatic normal mode.

For the slow mode, using the parameters discussed earlier, W may be approximated straight-forwardly and an analytic expression found when $|\bar{z}| \ll 1$ (e.g. Taylor expansion of W , here valid for the electrons) or $|\bar{z}| \gg 1$ (W may be expressed as an asymptotic series, valid to reasonable accuracy for the heavy C ions). Since for the H ions in the slow mode $\bar{z} \sim 1$, neither these approximations nor multi-pole expansions of W work well over the regime of interest (see Ref. [4] and references therein for further detail). Direct numerical solutions to Eq. (1) are shown in Fig. 1a for the fast and slow modes, lying at intersections of zero contours of the real and imaginary parts of $\epsilon(\omega, k\lambda_{D,e} = 1/3)$, where $\lambda_{D,e}$ is the electron Debye length (used throughout this Letter, $k\lambda_{D,e} = 1/3$ is typical of SBS experiments, although kinetic effects are only weakly dependent on this parameter). There are an infinite number of such intersections, each having different Landau damping decrements $\gamma = -\text{Im}[\omega]/\text{Re}[\omega]$; we refer to as “the slow mode” and “the fast mode” the least damped modes belonging to each class of mode.

Figures 1b-1e show the phase velocity and damping corresponding to the fast and slow modes as a function of T_i/T_e ; the slow mode is less damped than the fast for $T_i/T_e \gtrsim 0.2$, and is thus preferentially driven in this regime near the SBS threshold. It is interesting to ask: which species contributes most to the damping? In the

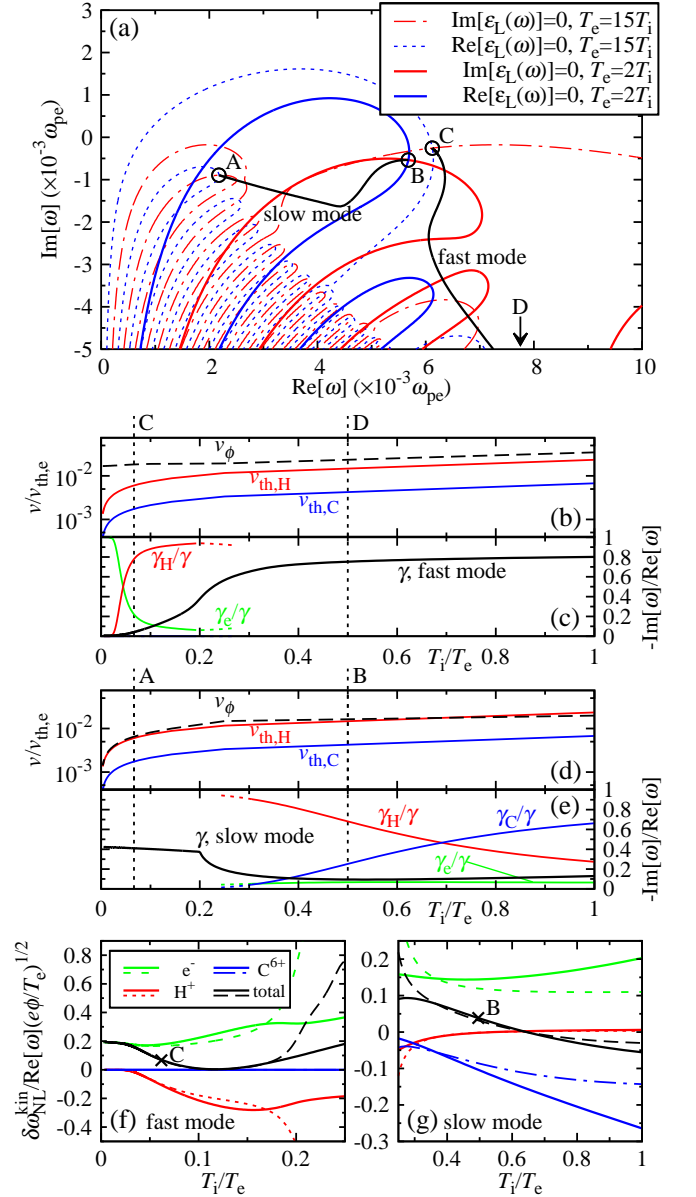


FIG. 1: (a) Contours of solutions to the slow and fast IAW mode dispersion relations for $k\lambda_{D,e} = 1/3$. As the ratio T_i/T_e increases from 1/15 to 1/2, the frequency of the slow mode moves from A to B and the fast mode from C to D. Below, the (b)/(d) mode phase velocities, (c)/(e) total damping decrement, fractional damping due to each species, and (f)/(g) kinetic nonlinear frequency shift (solid lines: $\epsilon_R = \text{Re}[\epsilon_L(\text{Re}[\omega], k)]$; patterned lines: $\epsilon_R = \text{Re}[\epsilon_L(\omega, k)]$).

resonant approximation (assuming $\text{Im}[\omega]/\text{Re}[\omega] \ll 1$), Eq. (1) may be solved to lowest order to yield the following analytic expression for the linear Landau damping, relevant to multi-species plasma waves:

$$\tilde{\gamma} = \sum_{\text{species}} \tilde{\gamma}_j \approx \beta_\gamma \sum_{\text{species}} \frac{1}{\tilde{v}_{th,j} \tilde{\lambda}_{D,j}^2} \exp(-\tilde{z}_j^2/2), \quad (3)$$

where $\beta_\gamma = \sqrt{\pi/2} \tilde{\omega}_R \tilde{k}^{-3} (\partial \epsilon_R / \partial \tilde{\omega}_R)^{-1}$, $\omega_R = \text{Re}[\omega]$ and

$\epsilon_R = \text{Re}[\epsilon_L]$ (ϵ_R is discussed later). Tilde denotes normalization to electron quantities $\lambda_{D,e}$, $v_{th,e}$, $\omega_{p,e}$, and T_e , as appropriate. For the electrons in an IAW, $\tilde{\gamma}_e/\beta_\gamma \approx 1$. Using Eq. (3), the fractional contribution of each species to the total damping is plotted in Figs. 1c and 1e (the restricted plotted range corresponds to the limits of the resonant approximation). Thus, across the regimes of physical interest (i.e. the more weakly damped regimes of each mode), the electrons contribute most to the damping of the fast mode for $T_i/T_e \lesssim 0.04$ and the H ions for $T_i/T_e \gtrsim 0.04$, while the H ions dominate the damping of the slow mode for $T_i/T_e \lesssim 0.7$ and the C ions for $T_i/T_e \gtrsim 0.7$.

The travelling potential ϕ of a plasma wave, propagating at the phase velocity v_ϕ , traps particles within the plasma with velocities close to v_ϕ . This trapping, in addition to suppressing Landau damping [8], leads to a nonlinear frequency shift $\delta\omega_{NL}^{kin}$ away from ω_R . Each species in the plasma makes a contribution to this effect, the significance of which is dependent upon the plasma parameters. Simple analytic expressions in which $\delta\omega_{NL}^{kin}$ is proportional to the square root of the potential amplitude have been derived in the sudden [9, 10] and adiabatic limits [10] of wave generation (these derivations are for the case of a Langmuir wave, but were shown to apply to IAWs in Ref. [5]), the latter being the more relevant to stimulated scattering processes and the conditions discussed here. Following this methodology, one finds for a multi-species plasma wave in the resonant approximation with Maxwellian distributions,

$$\delta\tilde{\omega}_{NL}^{kin} = -\beta_\omega |\tilde{\phi}|^{1/2} \sum_{\text{species}} \alpha_j \frac{1}{\tilde{\lambda}_{D,j}^2} \left(\frac{|\tilde{Z}_j|}{\tilde{T}_j} \right)^{1/2} K(\tilde{z}_j), \quad (4)$$

where $\beta_\omega = \sqrt{2/\pi k}^{-2} (\partial\epsilon_R/\partial\tilde{\omega}_R)^{-1}$, $\tilde{\phi} = e\phi/T_e$, α_j is a constant with a value dependent on how the species within the wave was excited (for adiabatic excitation, $\alpha_j = 0.544$; for sudden excitation, $\alpha_j = 0.823$ [10]), and the sign of the contribution of each species to the total shift is determined by $K(\tilde{z}_j) \equiv (\tilde{z}_j^2 - 1) \exp(-\tilde{z}_j^2/2)$.

Figures 1f and 1g plot Eq. (4) for the fast and slow wave, respectively ($\partial\epsilon_R/\partial\tilde{\omega}_R$ is evaluated numerically). Over the physically relevant (weakly-damped) range of T_i/T_e for each species, several features are apparent. For both the fast and the slow modes examined here, the positive frequency shift due to the electrons opposes and is of greater magnitude than the negative shift due to the ions, thus computationally lighter Boltzmann fluid models of electrons favoured in many past studies of IAWs would give incorrect results as they neglect electron trapping; the full kinetic behaviour of electron and ion species must be captured, as established in Ref. [11] for particle-in-cell simulations. One sees immediately from Fig. 1d that for the H ions of the slow mode, $K(z) \approx 0$ i.e. H ions make a negligible contribution to the nonlinear frequency shift [12], yet contribute most to Landau damping in the linear

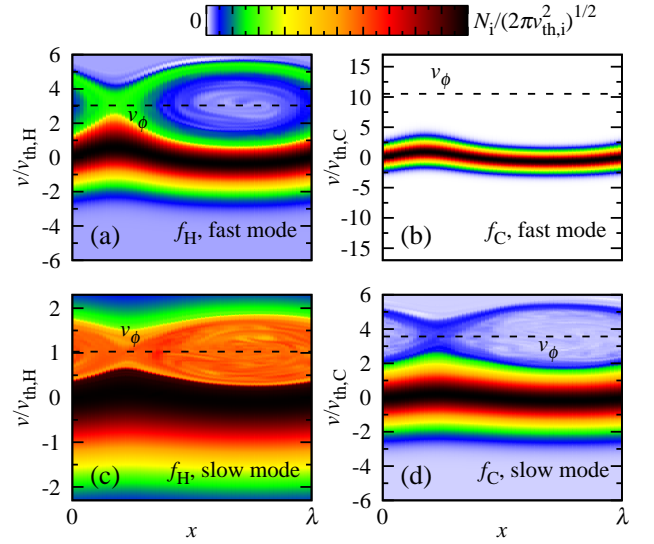


FIG. 2: Ion distributions from Vlasov simulations for the fast and slow modes after an undriven BGK-like mode has been established. Here, $\tilde{\phi} \sim 0.1$ for both modes.

limit; the C ions however make a significant contribution to the shift. In contrast, H ions in the fast mode provide a significant contribution to the shift, while the C ions with $v_{th,C} \ll v_\phi$ (see Fig. 1b) are negligible for both the nonlinear frequency shift and the linear Landau damping.

In the derivation of $\delta\omega_{NL}^{kin}$ in Refs. [9] and [10], it is seemingly ambiguous as to whether one should take $\epsilon_R = \text{Re}[\epsilon_L(\text{Re}[\omega], k)]$ or $\epsilon_R = \text{Re}[\epsilon_L(\omega, k)]$ (this is discussed in detail in Ref. [5]). Outside of the weakly damped region for each mode, as $\text{Im}[\omega]$ approaches $\text{Re}[\omega]$, Eqs. (3) and (4) differ greatly depending on the choice of ϵ_R made, giving results that are unphysical over certain ranges. However, within the weakly damped regimes for both modes, where the resonant approximation is valid, the choice of ϵ_R is of limited importance, as seen in Figs. 1f and 1g.

In order to investigate the physics described previously, the code SAPRISTI was used (described in Ref. [5]), which solves the full Vlasov-Poisson system for electrons as well as multiple ion species, retaining one dimension in space and velocity (1D1V). By restricting the simulation size to a single wavelength λ with periodic boundary conditions, processes such as IAW decay and modulational instability were prevented from occurring, allowing the precise analysis of the frequency of the nonlinear wave in isolation. In simulations, an IAW was driven at its linear frequency using a prescribed ponderomotive drive of a strength that ensured the growth was slow on the time scale of the ion plasma and ion bounce frequency, $\omega_{b,i} = k(\tilde{Z}_i e\phi/m_i)^{1/2}$. After the desired amplitude was reached (taking times of the order of $10^5 \omega_{p,e}^{-1}$), the driver was switched off and the IAW allowed to propagate freely. Measurements of particle distributions (Fig. 2) and frequency (Figs. 3c,d)

were made after a BGK-like mode [13] had been established due to trapping. The shift $\delta\omega_{\text{NL}}$ was determined by comparing the time-asymptotic state of the free IAW to an IAW of very low amplitude ($\phi \sim 10^{-4}$), and the amplitude to which the wave was driven was varied to determine the dependence of $\delta\omega_{\text{NL}}$ on ϕ (details of the signal processing techniques used are given in Ref. [5]). Two physically relevant, weakly-damped cases are presented here in detail: a fast mode, where $T_i/T_e = 0.07$, and a slow mode, where $T_i/T_e = 0.5$ (points C and B, respectively, in Fig. 1).

Figure 2 shows the distributions of the H ions, f_H , and C ions, f_C , for both modes. Figure 2c shows that while f_H is heavily modified, the particles are roughly evenly distributed across the trapping region. In contrast, the trapped C ions of the slow mode and H ions of the fast mode are concentrated at the separatrix, in agreement with the analytic result for the adiabatic distribution given in Ref. [10]. To confirm that all species in the IAW were driven adiabatically, the distribution of trapped particles was compared to various analytic models. Alongside Vlasov simulation results, the expected distributions of trapped C ions in the adiabatic and sudden excitation cases are shown in Fig. 3a, labelled f_{ad} and f_{sd} , respectively. The analytic calculations were repeated using the actual ϕ taken from simulations rather than assuming a sinusoid (and therefore including the impact of harmonic generation); the agreement between the adiabatic model and the simulation in this case is excellent for all species.

Harmonic generation in IAWs has been the subject of many previous studies. Solving the homogeneous cold-ion fluid equations for an IAW including its harmonics (see, e.g., Pesme *et al.* [14]) results in a first harmonic ϕ_1 driving a second harmonic ϕ_2 , scaling such that $|\phi_2| \sim |\phi_1|^2$, and a frequency shift of the fundamental $\delta\omega_{\text{NL}}^{\text{flu}}$ proportional to $|\phi_1|^2$. However, as in warm-ion plasmas studied here, significant additional terms increasing the coupling of harmonics arise due to the ion fluid pressure. Such effects are non-trivial to introduce in the case where the lighter ion species is neither light enough to screen the heavy species (in a similar fashion to the electron motion), nor heavy enough to oscillate in phase with the heavy species. In Fig. 3b, measured ratios $|\phi_2|/|\phi_1|$ for the fast and slow modes are shown. In fact neither fast nor slow modes show the scaling expected from a cold-ion fluid model. Single-species studies of harmonic generation have also been found to diverge from this model over a range of ion temperatures [5].

Figures 3c and 3d show the measured deviation in frequency $\delta\omega_{\text{NL}}$ from ω_0 as a function of ϕ (for Vlasov results, we measure $\omega_0 = \omega(\phi \rightarrow 0)$; for analytic calculations, $\omega_0 = \omega_R$). The observed trend of increasing frequency as a function of wave amplitude further supports the choice of the adiabatic limit of α_j in Eq. 4 for all species: using the sudden limit for the ions and an

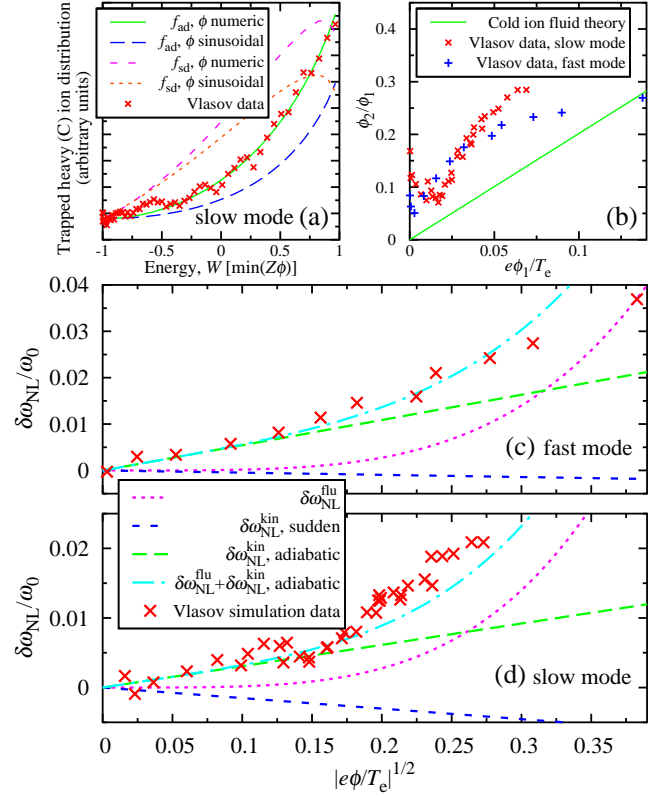


FIG. 3: (a) The trapped C ion distribution as a function of energy. (b) The relative amplitudes of the first and second harmonics of each mode. Below, the measured frequency shift of the (c) fast and (d) slow IAW modes compared to kinetic and fluid analytic calculations.

adiabatic limit for the electrons would imply an overall negative shift in frequency, contrary to what is observed in Vlasov simulations. From these results, it is clear that calculations of $\delta\omega_{\text{NL}}^{\text{kin}}$ from Eq. 4 match Vlasov results well for low ϕ , but under-estimate $\delta\omega_{\text{NL}}$ at higher amplitudes where harmonic generation is expected to contribute a further positive frequency shift. The fluid shift is also shown using a cold ion model. While not formally consistent, a simple linear sum of the kinetic and fluid frequency shifts shows convincing agreement with Vlasov results for fast and slow modes in both magnitude and ϕ scaling.

In summary, the rich and differing nonlinear behaviours of the fast and slow IAW modes of CH plasma have been presented in detail for the first time in regimes relevant to current ignition experiments. Good agreement between multi-species analytic calculations of the nonlinear frequency and highly-resolved Vlasov simulations across the most physically relevant regimes is observed. Across the more weakly damped regimes for each mode, the overall positive sign of the frequency shift of the fast mode, and of the slow mode for $T_i/T_e \lesssim 0.6$, imply (I) the electron dynamics must be sufficiently re-

solved for all T_i/T_e in order to accurately model nonlinear IAWs, and (II) both modes are susceptible to modulational instability of the type described in Ref. [15] over these ranges.

The authors gratefully acknowledge the helpful comments of B. I. Cohen. This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344 and funded by the Laboratory Research and Development Program at LLNL under project tracking code 12-ERD-061.

* email: chapman29@llnl.gov

- [1] N. B. Meezan *et al.*, Phys. Plasmas **17**, 056304 (2010).
- [2] D. H. Froula *et al.*, Phys. Plasmas **17**, 056302 (2010) and references therein.
- [3] D. S. Clark *et al.*, Phys. Plasmas **17**, 052703 (2010).
- [4] E. A. Williams *et al.*, Phys. Plasmas **2**, 129 (1995).
- [5] R. L. Berger *et al.*, under review for Phys. Plasmas., reference number 39701
- [6] S. C. Wilks *et al.*, Phys. Rev. Lett. **74**, 5048 (1995).
- [7] B. I. Cohen *et al.*, Phys. Plasmas **4**, 956 (1997).
- [8] T. M. O’Neil, Phys. Fluids **8**, 2255 (1965).
- [9] G. J. Morales and T. M. O’Neil, Phys. Rev. Lett., **28**, 417 (1972).
- [10] R. L. Dewar, Phys. Fluids **15**, 712 (1972).
- [11] C. Riconda *et al.*, Phys. Rev. Lett. **94**, 055003 (2005).
- [12] If instead of following the derivation found in Ref. [10] and Taylor expanding the H distribution around the phase velocity one finds the nonlinear part of the dispersion relation by numeric integration, the same result is obtained.
- [13] I. B. Bernstein, J. M. Greene, and M. D. Kruskal, Phys. Rev. **108**, 546 (1957).
- [14] D. Pesme, C. Riconda, and V. T. Tikhonchuk, Phys. Plasmas **12**, 092101 (2005).
- [15] R. L. Dewar, W. L. Kruer, and W. M. Manheimer, Phys. Rev. Lett. **28**, 215 (1972).